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Gas separation by adsorption: Technological drivers and opportunities for improvement

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Abstract

Chemical and petrochemical companies are increasingly realizing that their sustainable development critically depends upon development of new innovative processes that use more efficiently materials and energy. As overall separation/purification processes account for 40-60% of capital and operating costs, their amelioration can significantly reduce costs, energy use and waste generation by increasing profits. Gas separation by adsorption technology is a well-established unit operation in chemical and petrochemical industries due to its efficiency for dealing with a large range of gas separations including impurity removal, gas purification and separation in recycle streams. The technology is far from being mature and opportunities to expand its domain of applicability and improve its efficiency are high in a context where better understanding of physical phenomena and technological progress in materials and engineering research are integrated. Major contribution for innovations in gas separation by adsorption technology relate to the discovery of new adsorbents with better separation characteristics coupled to process development and its optimization using multi-objective and multi-domain numerical approaches. This short review identifies technological gaps and drivers for accelerating the development of industrially important gas separations by adsorption.

1. Introduction

The nanoscale manipulation of porous materials [1–6] opens perspectives for their design with controlled structures and properties needed in many industrial gas separation processes [7]. A clear trend observed during the recent years is the synergy between the progresses made in this field and those in computational technologies such as evolutionary computational modelling, computational chemistry, molecular modelling and process design and optimization based on multi-objective multi-domain paradigms. The coupling of experiment with modelling at various time and length scales based on advances in software technology (Knowledge Discovery in Databases [8,9], Artificial Intelligence [10,11], Multi-scale simulation [12–14], Structure-Activity[15] and Structure-Function relationships [3], Molecular Simulations [16–20], Process Simulation & Optimization [21–25]) and synthesis by design of novel Nano-structured materials allows identification of pathways for rapid progress in gas separation by adsorption technology. Another important aspect of adsorbent research is the shaping of adsorbent materials [6,26–29] into micron-length and macroscopic scale objects like pellets extrudes or monoliths. The shaping process responsible for mass transfer kinetics highly affects the performance of the separation unit. The optimal shaping recipe carried out through an iterative shaping and consecutive experimental characterization approach before process evaluation in bench-scale pilots. The final validation of the newly developed process for a given gas phase separation is achieved in pilot plant-scale for commercial flow sheet confirmation. Several recent reports on gas separation applications using this technology indicate trends of improvement in this field. Due to space limitation, we primarily consider peer-reviewed literature, referring to patents only when the peer-reviewed literature lacks such information.

2. Gas separation by adsorption: accelerating innovation through numerical simulations

The Separation/purification of industrial gases in the 5-200 t/day range by adsorption technologies, e.g., pressure swing adsorption(PSA) [21,24,25,30] and vacuum swing adsorption (VSA) [31,32] show a faster growing rate than the conventional cryogenic-based separation due to their up to 25% reduced cost of produced gas. The VSA/PSA is the gas separation process of choice for bulk gas production from feeds in which the produced gas presents above 10% v/v of the gas mixture. The use of temperature swing adsorption (TSA) industrially relates mainly to front end purification applications like fluid drying or eliminating of CO2 and secondary trace compounds from air prior its cryogenic distillation. During the last years, several concepts based on TSA or hybrid PTSA cycle schemes have been proposed [33–35] including applications such as direct CO2 capture from air [36–38] or CO2 capture from different feed gases[39–42]. The estimated cost for CO2 capture in these TSA-based purification processes concepts remains high for large-scale applications [43,44] and the difficulty of their implementation is mainly due to the low thermal conductivity of the adsorbent packed in an adsorbent bed and consequently to the very long cycle times. Although there is still considerable room for improvement in the design and operation of PSA/VSA and TSA processes, most gains in unit performance will likely come from the development of new and improved adsorbents. With increasing environmental and energetic concerns worldwide, porous materials [2,45–49] used as adsorbents in gas separation technologies are becoming even more important for the separation of polluting species, the recovery of useful ones and their use in sensor and catalyst developments. The Nano-porous materials fall into the category of large microporous and mesoporous materials with pore dimensions in the 0.3 to 30 nm range. The design, synthesis and processing [6,26,28] of these materials into adsorbents is a far more challenging task than the obtaining of dense materials because they are metastable phases in the sense that are created by interrupting the kinetics of single-phase assemblies. [12]

The development of new adsorbents with improved selectivity, stability, mass and heat transfer characteristics due favorable formulation and shaping has been the main factor of cost reduction and innovation in separation technologies by adsorption during the last decade. The introduction of a new adsorbent implies the redesign of the separation process configuration in order to optimize the performance of a separation unit. The experimental effort and the cost for the development of improved PSA, VSA or TSA separation units are relatively high if relying solely on costly experimental programs involving synthesis, structural characterization of porous material followed by their conversion in improved adsorbents and the final performance assessment in pilot-scale plants. In this context, the approach in which the modelling protocols are used for generating libraries of “virtual” [20,50,51] Nano-porous materials and the ability to predict their properties prior to experiment for pre-selecting new potential adsorbent structures, followed by process optimization simulations can effectively reduce the cost and time of the research for novel adsorption-based separation processes.

The ability to model, simulate and predict the behavior of Nano-porous materials at different length and time scales is a critical issue for the successful development of new adsorbents not only for the gas separation by adsorption or separation technology but also for a large number of industries that utilize these materials in their production cycles. The field of materials science and engineering is evolving very rapidly due to the computationally empowered materials discovery [52–54], development and deployment. In this context, the Materials Genome Initiative (MGI) [46,52,55] is aiming the enhancement of the fundamental understanding of materials science by providing the information needed for accelerating the development of new Nano-porous materials. It also allows connection into a much broader model-based engineering innovative process [21,22,56] that links manufacturing with design via advanced process-structure-property models [15,57] in an integrated

computational environment. This process involves integration of information across different length and time scales [12],[34,58–61] for relevant materials phenomena and enables concurrent analysis of manufacturing [29], [47], [15], [51], [48], [52] process and material properties within a holistic framework.

As PSA/VSA processes are relatively more complex than the TSA ones in the following, only the first ones are explicitly mentioned intending that the same reasoning apply also to TSA process. The main advantage of PSA/VSA technology [64], [22], [65] is their great flexibility that pays for the process complexity, which is still one of the major barriers for introducing the technology in new industrial applications. During last years, a continuous progress in process engineering has improved the productivity and recovery of PSA/VSA units [32,66], [67,68]. Between these advances, the most challenging one is the development of cyclic strategies based upon accurate knowledge of the dynamic behavior of adsorbent/gas systems [6,69,70][1,70] that can improve the performance indicators of the PSA/VSA units. In order to accelerate the design of improved PSA/VSA units for selected gas separations, the integration of model based, and concurrent numerical approaches of the process in numerical workflows together with the adsorbent discovery as schematically reported in Figure 1 is exceedingly important. The numerical workflow comports a number of “numerical filters” reported in the upper part of Figure 1 and used for rapid screening of potential solutions for a selected separation. The experimental phase reported in the lower part of Figure 1 composed of several steps focuses on the selected number of solutions only.

This numerical approach allows not only to revisit existing well-established gas separation by adsorption technologies but also to develop novel PSA/VSA separation schemes for industrially important separations such as olefin-paraffin, diene/olefin, N2/CH4, CO2/CH4, CO2 removal from industrial gas streams and other difficult hydrocarbon separations. For example, the separation of light olefins from gases produced by pyrolysis of hydrocarbons is a major issue for the cost effectiveness of the olefins production plants. Another example related with ethylene production based on Oxidative Coupling of Methane (OCM) consists in gas separation and recycling from the OCM reactor using PSA technology. In the xylenes isomerization unit operating under a hydrogen partial pressure of 25 to 35 bars in which the recycled gas contains many impurities, such as benzene, toluene and xylenes the PSA unit allows to recover the p-xylene and improve the overall performance of the unit. In the aniline synthesis process based on Nitrobenzene hydrogenation, the recycle loop containing hydrogen rich complex gas mixture that is hard to separate and therefore huge quantities of hydrogen are lost by purge of recycle gas a PSA separation unit improves the performance of the unit.

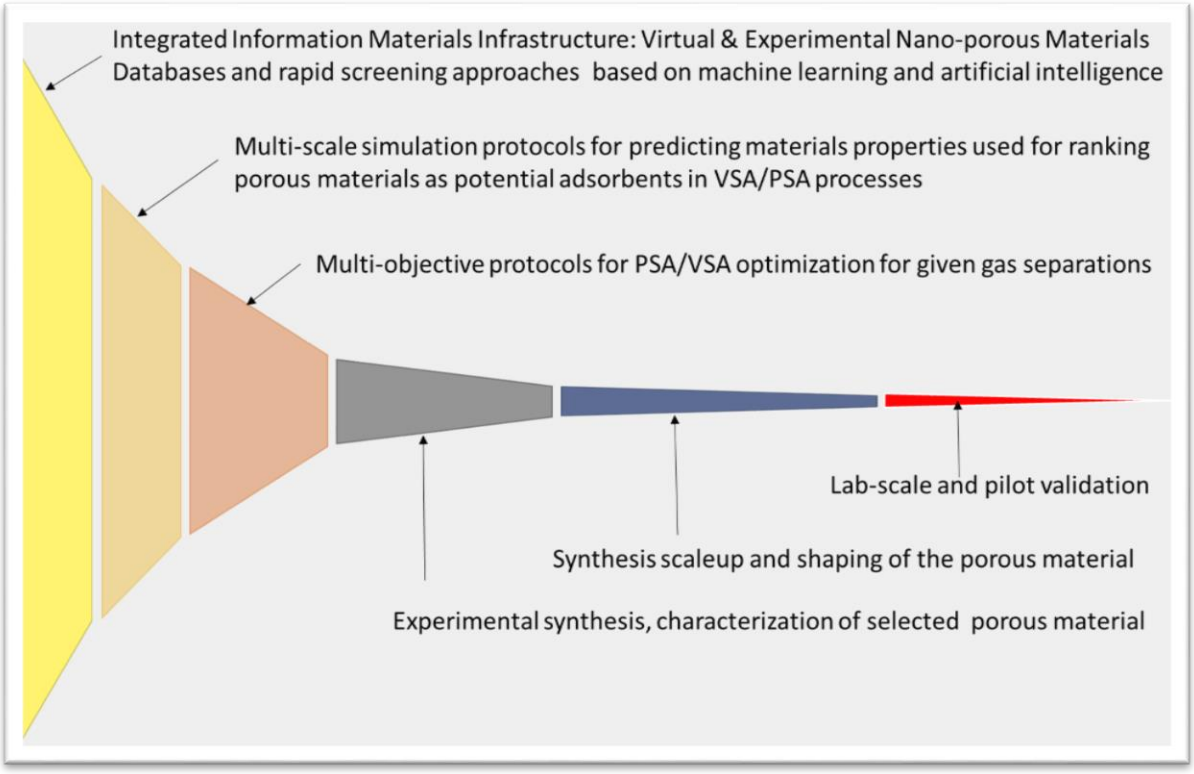

Figure 1: Schematic representation Nano-porous materials discovery coupled to PSA/VSA multi-objective process optimization for reducing the time and effort of development of new solutions

In the following, we report recent advances in a number of emerging technologies as part of the numerical workflow reported in Figure 1 that when integrated with the experimental developments in the field of gas separation by PSA/VSA technology could accelerate the improvement of several conventional gas separation by adsorption applications and accelerate the development of new ones.

2.1. Knowledge Discovery in Databases

Massive amounts of data generated each year for Nano-porous materials as a small part of the MGI including almost any type of digital information, obtained whether from experiment or computation imply the development of dedicated approaches to cope with knowledge discovery in scientific data [8,11,71–73]. The natural evolution of MGI was towards data exploitation through a Materials Data Infrastructure [52,73–75] (MDI) giving rise to agreements from scientific communities for developing basic guidelines known as ‘’FAIR Principles’’ [11] for the data management that should be: Findable, Accessible, Interoperable, and Reusable. Dedicated tools embedded in MDI platform allow for the capture, processing, cleaning, dissemination and knowledge discovery in data[9,76–78], enabling their increased reuse by a wide research community going from materials scientists to chemical engineers that use the materials for improving their process technologies and final products. In this context, the numerical screening [12,13,46,48,72,79–82] of target properties of adsorbent materials for well-defined gas mixtures as well as their potential improvement through the design rules for guiding the synthesis of new Nano-porous materials opens perspectives for rapid exploration of new classes of porous materials [3,5,46,47,49,83–87]. The generation of design rules for selecting the appropriate material is possible because of the digital description of both materials and processes and their combination in model-based reasoning in the conceptual stage of PSA/VSA process development for a selected gas separation application.

Another relevant activity for accelerating developments in PSA/VSA technology relates to the construction data warehouses [76,88–90] or data lakes containing structured information on gas separation properties of Nano-porous materials and adsorbents. The stored information relates to the intrinsic structural features and properties of the Nano-porous materials or adsorbent properties such as their specific heat capacity, as well as information related to pure gas adsorption and multicomponent gas adsorption of selected gases and gas mixtures on Nano-porous materials or adsorbents including thermodynamic and kinetic information. The classification of data extracted from experiments and their organization into thematic groups known as data marts obtained through data mining algorithms and several existing data analytics techniques [75,78,91,92]. These include beside classical analysis tools, statistical methods, deep learning (DL), artificial neural networks (ANN), data mining (DM) and heuristic techniques, expert systems (ES) [71], case-based reasoning [93] (CBR) and inductive logic programming (ILP) [85]. Knowledge extraction from data intends their visualization, classification, prediction, generalization, correlation and decision validation rules together with the possibility to estimate data quality as an essential element in the context of prediction quality and its reusability [80,94]. Quantitative estimation of data quality includes data validation (for computationally derived data), verification, uncertainty, accuracy and sensitivity [90,95].

2.2. Multi-scale Modeling and Simulation Tools

In the recent literature, the concept of multi–scale modelling and simulation [12–15,40,96] appears as a general trend for improving the understanding and the performance of several materials-based technologies. In the case of gas separation by adsorption, multi-scale modelling represents a combination of several computational approaches. These range from the materials design [59], [85,97–104], synthesis and shaping [6,26,27,29] in desired geometries (pellets, extrudes or monoliths) by coupling modelling to experiment at various length and time scales in studies of complex Nano-porous materials like zeolites or other inorganic or hybrid Nano-porous materials. In this field, experimental studies have preceded by far the theoretical ones. During the last decade, however, computational chemistry has had a favorable impact almost in all branches of crystalline microporous materials research ranging from phase determination to structural characterization and property prediction [59,79,105–107]. An important effort consisted in developing simulation tools for describing thermodynamic and transport properties of confined fluids in the nanometer-scale pores together with a realistic representation of adsorption phenomena [5], [78], [91],[95][98-111].

A critical challenge in developing successful nanoscale-controlled materials is the development of reliable simulation tools to guide the design, synthesis, including in operando monitoring of adsorption phenomena using X-ray tomographic imaging techniques combined with computed tomography (CT) methods allowing for multi-dimensional spatial information referred also as digital adsorption [112] and testing of the Nano-porous materials [2,83,85,99,101]. In recent years important progress has been reached in building fast computational software that reliably predicts the chemistry and physics (structures and properties) as a function of conditions (temperature, pressure, concentrations) and time. In addition, approaches that allow the application of “de-novo” design procedures for synthesizing crystalline porous materials as zeolites, Metal-Organic Framework Materials (MOF) and other Nano-porous materials for specific separation processes [69], [13,53,83,113,114]. In order to respond to the engineering demand for new concepts for PSA/VSA technology improvement, it is necessary to extend numerical approaches from Quantum Mechanics (QM) scale to engineering design and process simulation by a succession of scales, where at each scale; the parameters are determined by averaging over the lower scale [13,58–60,71]. This will allow the use of first-principles simulations to contribute to solving engineering problems. Despite the progress in first principles electronic structure theory, these calculations remain far too slow for studying the overall phenomena in Nano-

porous materials applications to gas separation by adsorption [5,40,80,97,115–117]. For this reason, during the last years have been developed and used specialized adsorption Force Fields (FF) that faithfully represent the structures and adsorption properties of porous materials [107,118–122]. Molecular simulations allow the generation or complementing of experimental multi component adsorption data in crystalline and amorphous Nano-porous materials [20,70,123].

The capability to model materials shaping in adsorbents and their manufacturing process will further enhance the design capacities of improved adsorbents [1,6,26–29]. In addition, the 3D reconstruction of adsorbers filled with adsorbent beads or monoliths made of Nano porous materials with realistic representation of the different porosities and their distribution is essential for improving models used for the prediction of mass and heat transfer [4,70,124,125] over a variety of time and length scales used in separation process design [114].

2.3. Process Design and Multi-Objective Optimization

The introduction of concurrent engineering has led not only to reduced time to market but also to an integrated approach of product and process development. This last aspect supported by multi-objective optimization approaches [126–130] has a strong potential for achieving better design solutions taking into account all relevant parameters from both adsorbent and process simulation domains that contribute directly or indirectly to globally optimal solutions. It is important to emphasize that the use of figures of merit to select adsorbent materials for specific separations has limitations and the complexity of VSA/PSA processes requires process optimization to rank properly novel materials[131]. The development such approaches [30,132–135] based on numerical simulations and knowledge extraction from data implies the systematic validation of the parameters used for characterizing adsorbents and the detailed process simulation [97,136–139]. In this context, the accuracy and data consistency check of primary data, from experimental or simulation sources[3,63,72,85] before their transformation through simulation protocols and combination with other data sources is of principal importance. The introduction of uncertainties in the process design offers a significant potential for a higher level of reliability and safety margin in the optimization of the production process as robust optimization [128] approaches recently have gained attention within the engineering and scientific communities since many real-world optimization problems in numerous disciplines and application areas, contain uncertainty. This uncertainty is due to errors in measurements simulated properties, or difficulties in sampling.

The optimization of cyclic adsorption processes is inherently complex due to the dynamic and transient behavior of cyclic mass and heat transfer as well as the tight relation between adsorbent characteristics adsorber configuration, operational conditions such as cycle time steps and their scheduling [21,24,138,140–142]. The prediction of the adsorption bed dynamics behavior requires the simultaneous solution of a set of coupled partial differential equations (PDEs) representing material, energy, and momentum balances over the adsorber with the appropriate boundary conditions. The simultaneous solution of a system of PDEs is tedious and time consuming due to the need for reaching the cyclic steady state before estimating the performance indicators of the separation unit. The simulation of a PSA/VSA process implies the definition of a cycle structure followed by the estimation of the performance indicators. For the selected cycle, the entire step times, blowdown pressure, and flowrates of rinse and purge steps should be determined. In most cases, the definition of the cycle has to be done under certain constrains like combining it in a multiple column configuration. Other constraints can result from the availability of gas to the purge step, the continuous utilization of vacuum pump for blowdown. The availability of gas to the purge step can also proceed from a depressurization step (provide purge) or from a pre-stored amount in a tank. The estimation of performance [30,132,143] indicators of PSA/VSA separation unit show a strong coupling between the

process design and adsorbent selection with an increasing complexity of the PDEs resolution by the Cyclic Steady State (CSS) condition that should be met. The multi-objective optimization of a PSA/VSA system [132] represents a clear advantage over single objective optimization approach for the identification of process configurations on the Pareto frontier of which have equivalent unit performances but differing on the adsorbent properties, adsorber design and operational conditions. However, from the point of view of the computational power, multi-objective optimization is significantly more computational demanding. In order to reduce the simulation time a key idea is to replace the process simulators used in the multi-objective approach codes by fast emulators that mimic their behavior but run hundreds or thousands of times faster.

2.4. Adsorbent Materials Characterization

Adsorbent materials characterization [6,46,99,144] consists in several experimental techniques classified as static or dynamic ones used to extract information on adsorption thermodynamic properties of pure and gas mixtures in well-characterized porous materials for feeding theoretical and simulation approaches used for rapid data generation for gas adsorption in crystalline adsorbent materials. A major methodological development has been the introduction of fast DFT based methodology [99,144] for describing fluid properties in microporous heterogeneous adsorbents generalized to regular as well as amorphous nanomaterials and also to mixtures of regular and amorphous structures. The results of this approach are comparable to the recently developed simulation methods such as histogram reweighting Monte Carlo sampling allowing a significantly more accurate determination of phase coexistence properties than previously available techniques. These methods enable the location of critical points for strongly interacting fluids in confined pores.

Rapid experimental characterization techniques are necessary for screening large libraries of Nano-porous materials to identify potential adsorbents for PSA/VSA separations. Often the synthesis of novel materials carried out in small batches of approximately 100-200 mg is followed by a series of structural porosity, morphology and materials stability characterizations using several techniques including spectroscopic and diffraction methods before the synthesis scale-up. In order to rapidly asses the performance of new adsorbent materials for a PSA/VSA application the Zero Length Column (ZLC) technique [59], [132]–[134] allows for the estimation of mass transfer kinetic properties under low flow conditions, as well as the measure the full adsorption isotherm and Henry law constants in a single experiment using less than 10 mg. The great flexibility of the technique, involves some limitations related to the quality of data for given systems. The results obtained with the ZLC technique are very useful for rapid screening of adsorbent materials and for selecting the most promising ones for further investigation. Gravimetric measurements of adsorption isotherms of pure gases as well as Volume-Gravimetric, and Volumetric-Chromatographic for mixed gases measurements on newly developed Nano porous materials in the range of conditions relevant for the separation of interest are used for the final section of new adsorbent materials.

An important aspect of adsorbent material characterization is the combination of experimental characterization techniques with the ability to predict accurate and consistent data over a wide range of temperatures and loadings starting from few experimental data through coupling to molecular simulations. Methods for rapid prediction of gas adsorption on different classes of Nano porous materials represented by realistic details of pore structure and Pore size Distribution are essential for the design of optimal adsorbents. The description of the experimental data by a validated approach for predicting multi-component adsorption [123] in newly developed adsorbents will enable realistic simulations of PSA/VSA processes and efficient optimization of their performances.

2.5. Synthesis Scale-Up and Materials Processing

The synthesis [6], [27] and processing [135], [136] of selected adsorbent (nanostructured porous) materials of macroscale shapes (pellets, extrudes, monoliths or supported structures) [1,4,6,26,28,29,115,147,148] that can be used in industrial applications respecting detailed requests in line with the characteristics of the separation process are very challenging and offer important opportunities for radical innovations in gas separation by adsorption technology. The synthesis space is vast and is mainly controlled by mass transfer and reaction kinetics resulting in self-assembled structures whose stability depends on the presence of structuring agents as well as the stabilizing interaction of the solvent. The experimental exploration of the configurational space of possible porous materials is practically impossible due to the large number of parameters and their combination. Numerical generation of virtual porous materials [46,51,82] constructed through numerical assembling protocols defined at atomistic and cluster level becomes simple and can lead to the definition of design rules to guide experimental synthesis. This approach can be further extended to the estimation of processing parameters by simultaneous independent synthetic methodologies of hierarchical structure on different length scales.

Hierarchical structure design [45,146,149] based on a nanoscale molecular assembly achieved by a multi-dimensional control of function and properties has important implications in materials synthesis and related application technologies. Three-dimensional patterning and periodicity give the best surface area/volume dimensionality, optimum useful access space, and nanoscale control of structure and properties. Reported high surface area materials (up to 5,000 m^2/g) are metastable phases. Similar to zeolite structures, Metal Organic Frameworks (MOFs) [48,53,107,150] built from either tetrahedral or octahedral building blocks contain 3D Nano-scale porous channels and ultra-high specific surface areas, with potentially wide applications in asymmetric catalysis and chemical selective separation. Large libraries [53,72] of these materials obtained by building extended analogues of metal clusters with multi-dentate linkers such as carboxylate or poly-pyridine, according to a strategy that allows the realization of the most porous and thermally stable frameworks yet reported. Measurement of gas adsorption isotherm on evacuated derivatives of porous MOFs evidence the existence of accessible channels having a structural integrity and organization. The crystal engineering of coordination polymers enables the gain of control of the topology and geometry of the networks formed through a judicious choice of ligand and metal precursors and numerical simulations can estimate their chemical stabilities.

Activated alumina, silica gel and activated carbon are amorphous porous materials [28,145,151–154] shaped in beaded form that are used as adsorbents in industrially important gas separations. The possibility to adjust of the adsorption properties of these materials by modification of their pore size distribution (PSD) [151,155–157] or the nature of the active sites in the pores by specific post treatment or functionalization protocols allows their use in a wide range of gas separation by adsorption applications. In addition, these materials are being developed as basis of hybrid (amorphous-crystalline) porous materials. The incorporation of available crystalline Nano-porous materials in silica-gel matrix with controlled PSD allow the modification of their adsorption properties and their further assembling in beaded forms. The shaping protocol has a strong effect on the performances of adsorption-based separations by affecting the mass transfer rate of gases from and to adsorbent particles, particularly those used in PSA and VPSA separation units. By increasing mass transfer rate, the cycle time becomes shorter and the power consumption lower with consequently higher productivities and process efficiencies for PSA/VPSA processes [125,158,159]. This is particular relevant in Carbon Capture applications [160]. The shaping protocol directly affects the pellet porosity and its distribution by influencing macropore diffusion of gases within the adsorbent bead or pellet.

Lowering of the binder content may result in increased porosity and improved mass transfer rate. However, as it is also desirable to use adsorbents with high attrition resistance it may also result in fragile adsorbent particles that will collapse during cyclic operations. On the other hand, increasing the binder content will strengthen the adsorbent particle, but may create a particle that is too dense resulting in a poor mass transfer rate. Revisiting of the shaping process used to fabricate adsorbents with improved mass transfer properties by combining in a Design of Experiments (DOE) the shaping and characterizing protocols with the numerical simulation ones is opening perspectives for accelerating adsorbent optimization [31]. The numerical protocols consist in generating virtual pellets made of adsorbent materials and appropriate binders having controlled porosity and pore connectivity with final estimation of the mass transfer properties by numerical simulations. The numerical optimization of the virtual pellet "structure" allows for generation of design rules that can orient the experimentalist to shorten the time and apply rational approach for adsorbent mass transfer characteristics improvement [4].

3. Final remarks

Advances in computational power, computing infrastructures, new storage hierarchies and improved algorithms for dealing with more realistic complex multi-scale models supported by modern data science techniques, including machine learning and artificial intelligence, provide new opportunities for rapid progress in gas separation by adsorption technology. The use of physics-based understanding of Nano porous material adsorption properties combined with data-driven techniques have already demonstrated the ability for a rapid and efficient means to augment materials discovery, design, and deployment for adsorbent manufacturing.

The capability to model materials processing and manufacturing process and integrate these models in a numerical workflow with PSA/VSA process simulations using a multi-objective optimization approach will enhance the design capacities for selected gas separations and accelerate the development of new gas separations applications based on the paradigm of model-based engineering.

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∗ papers of special interest

** papers of outstanding interest

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